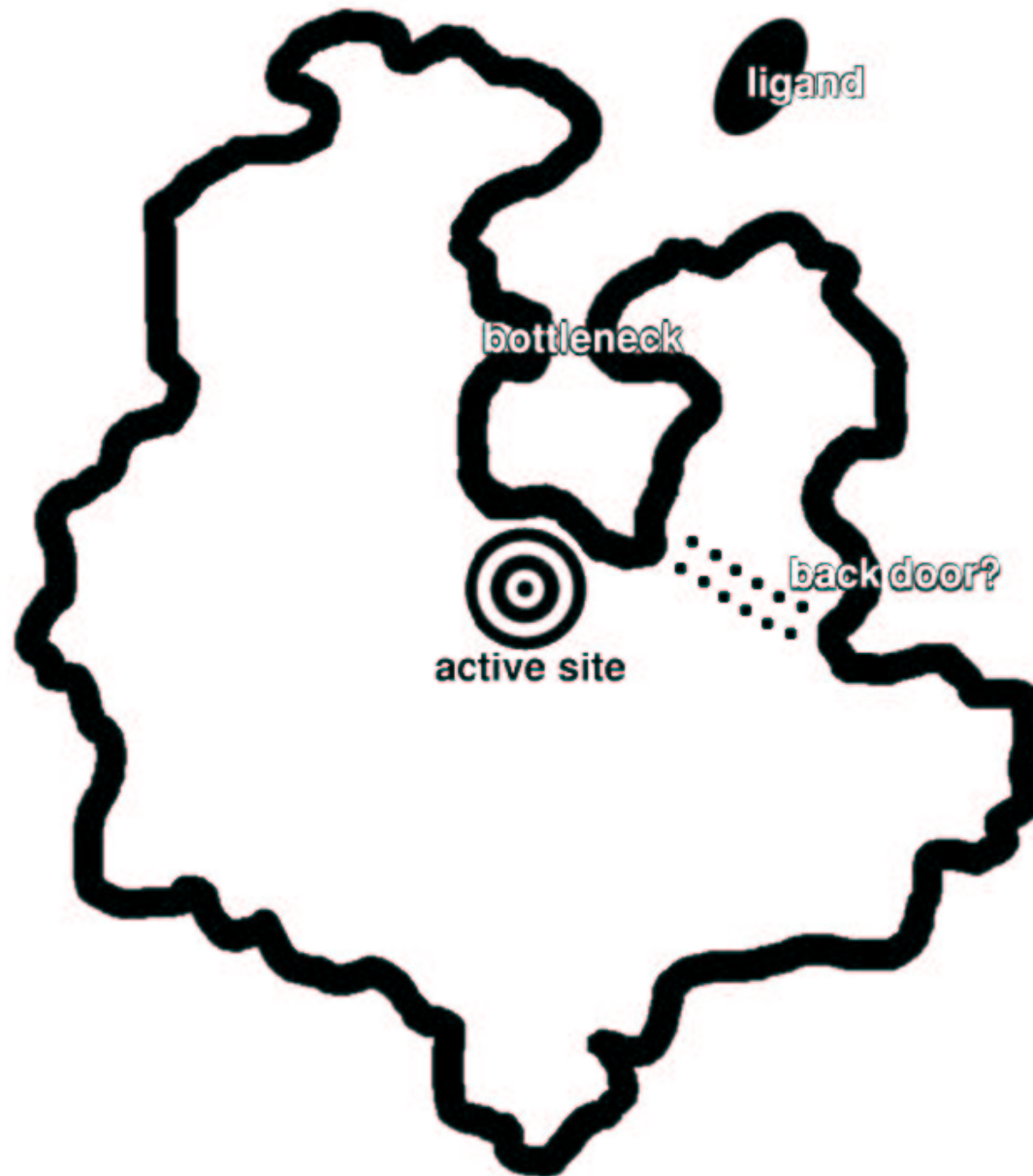


Simulations of molecules and processes in the synapse

Kaihsu Tai

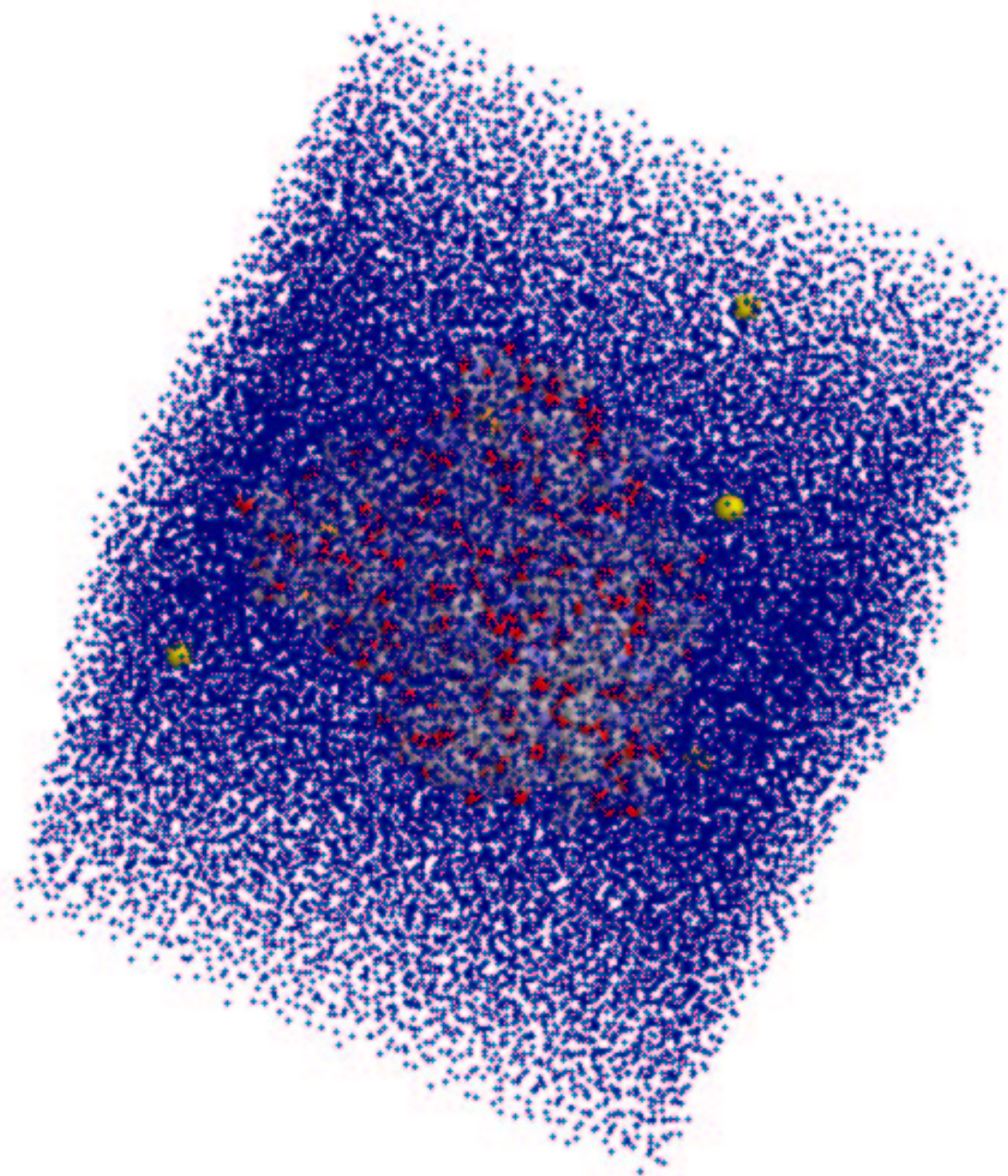


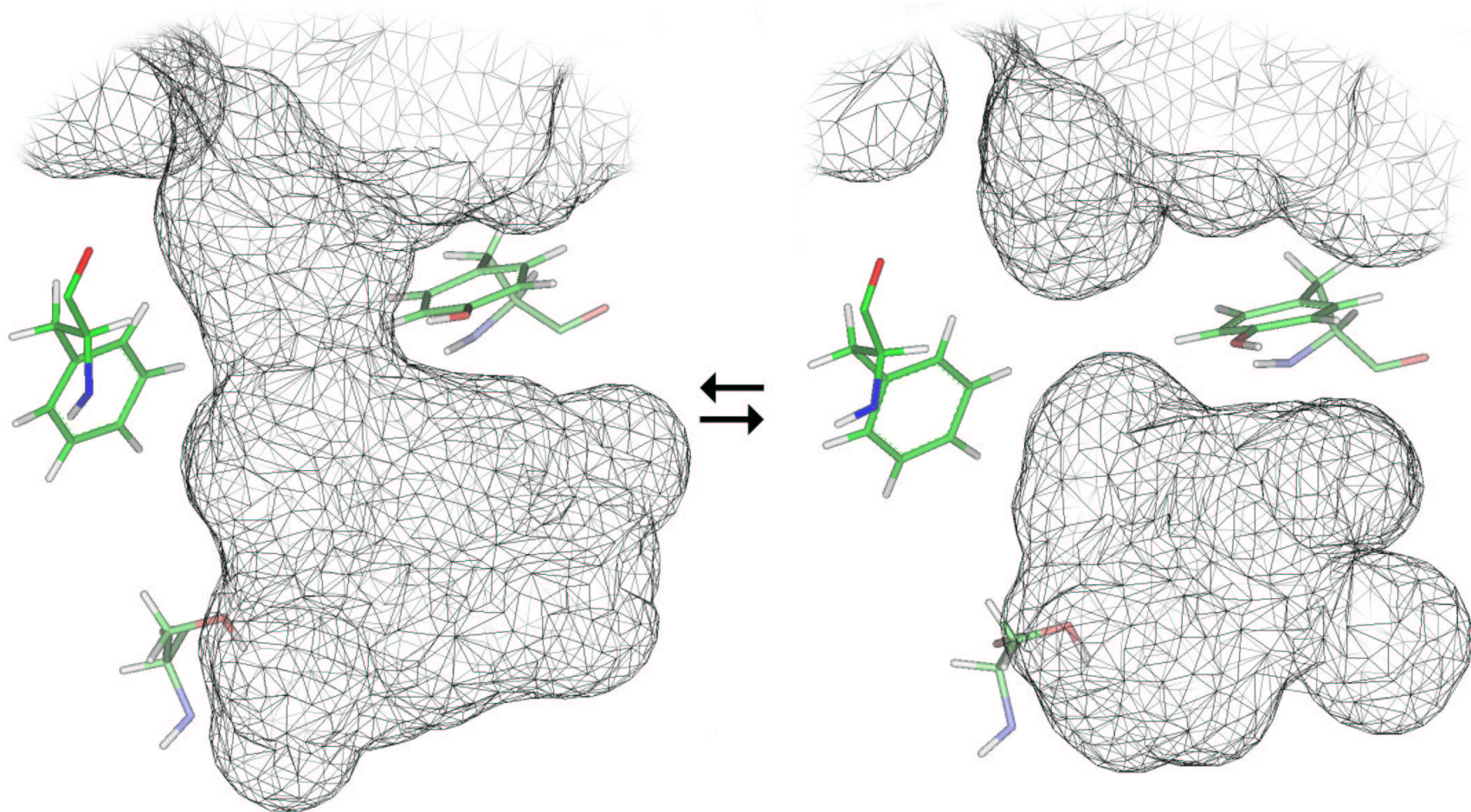


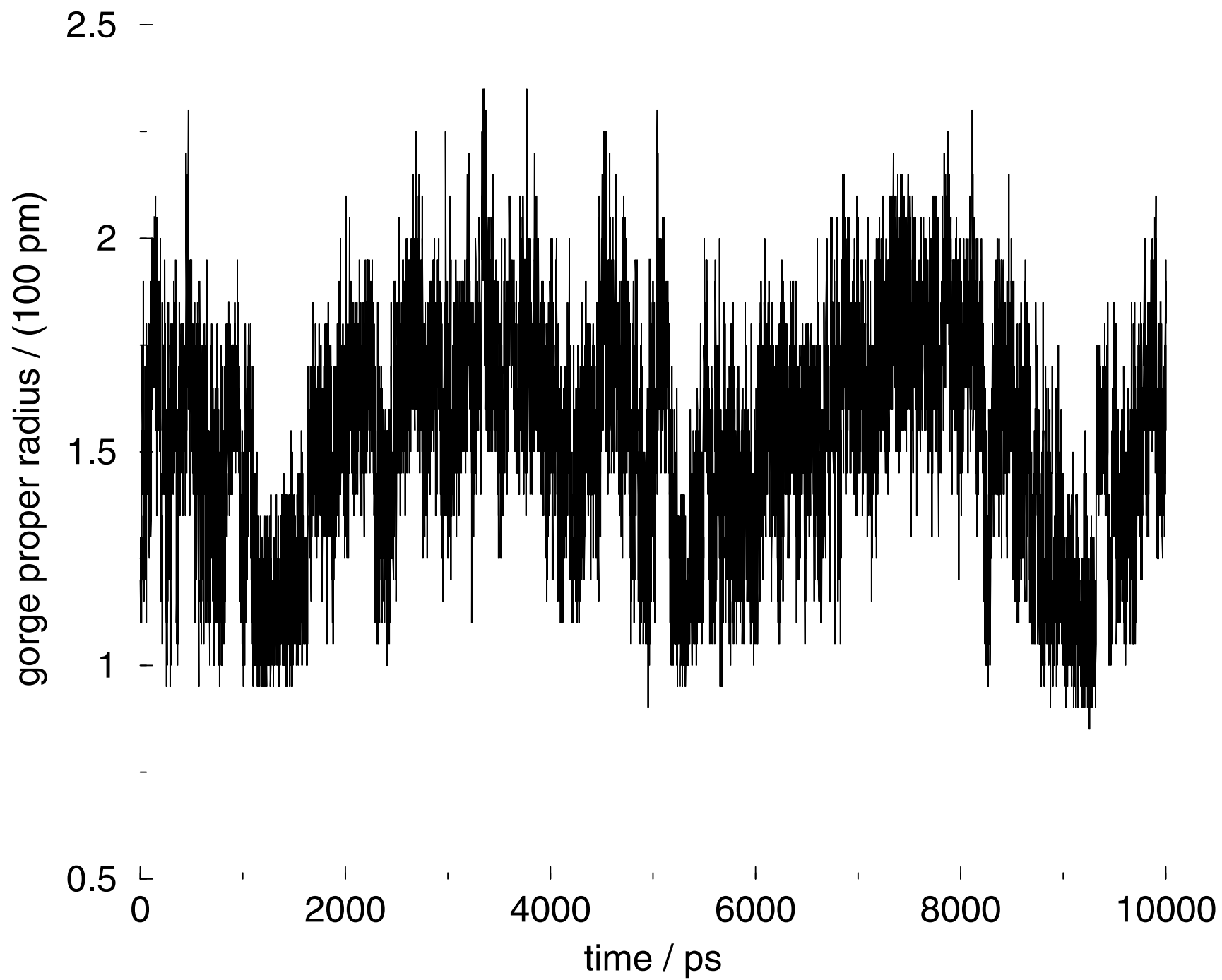
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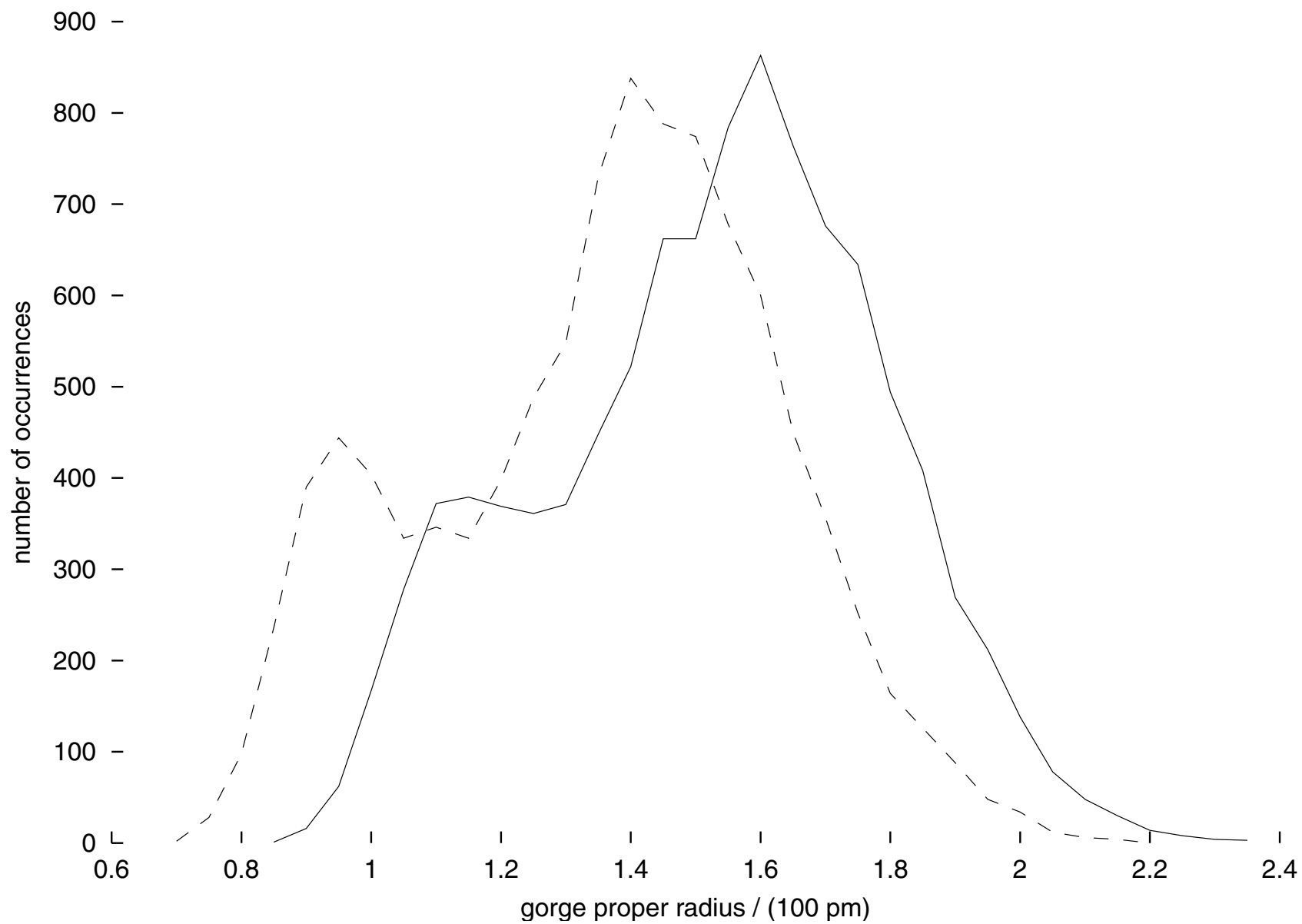


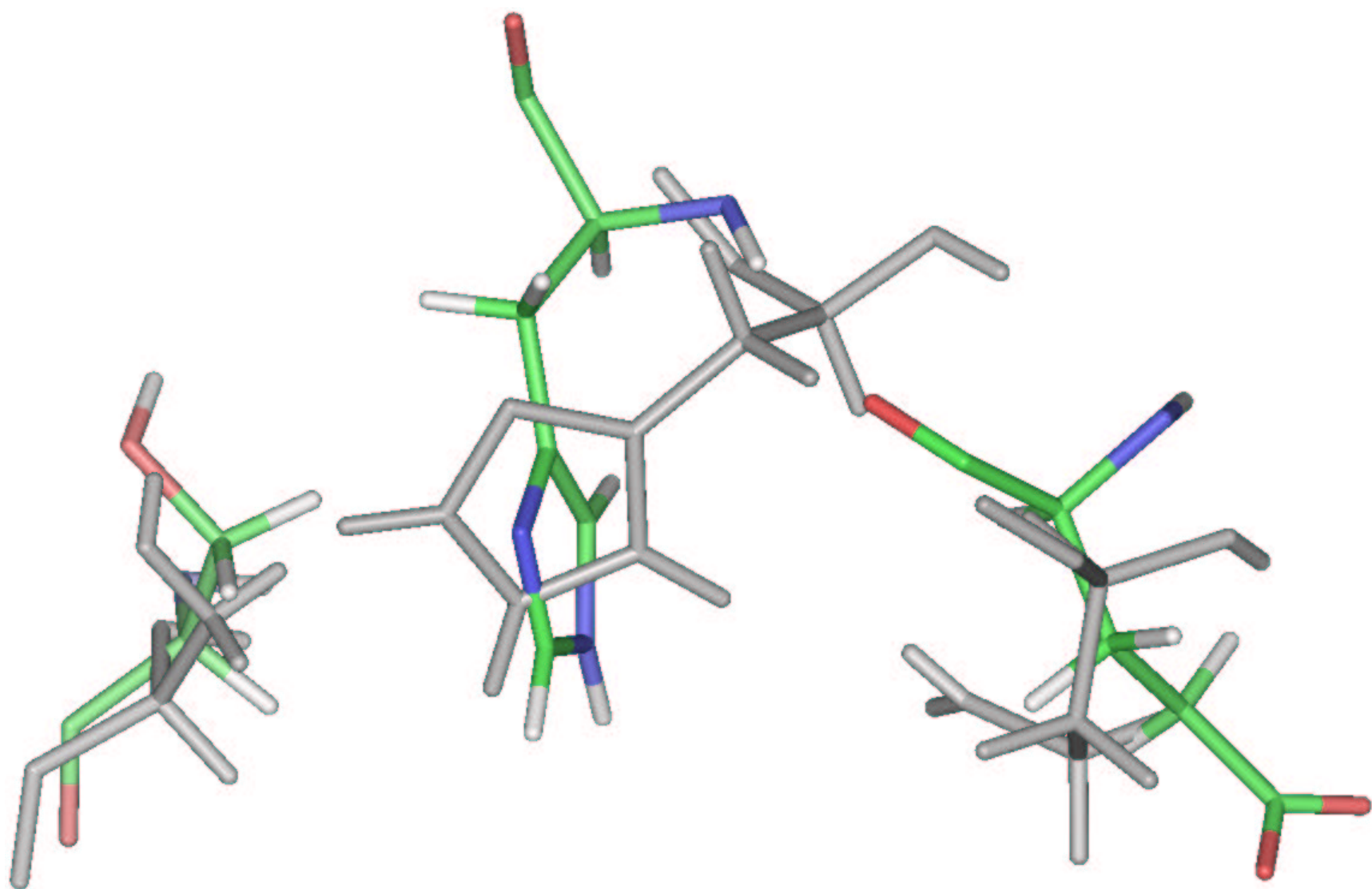
acetylcholinesterase





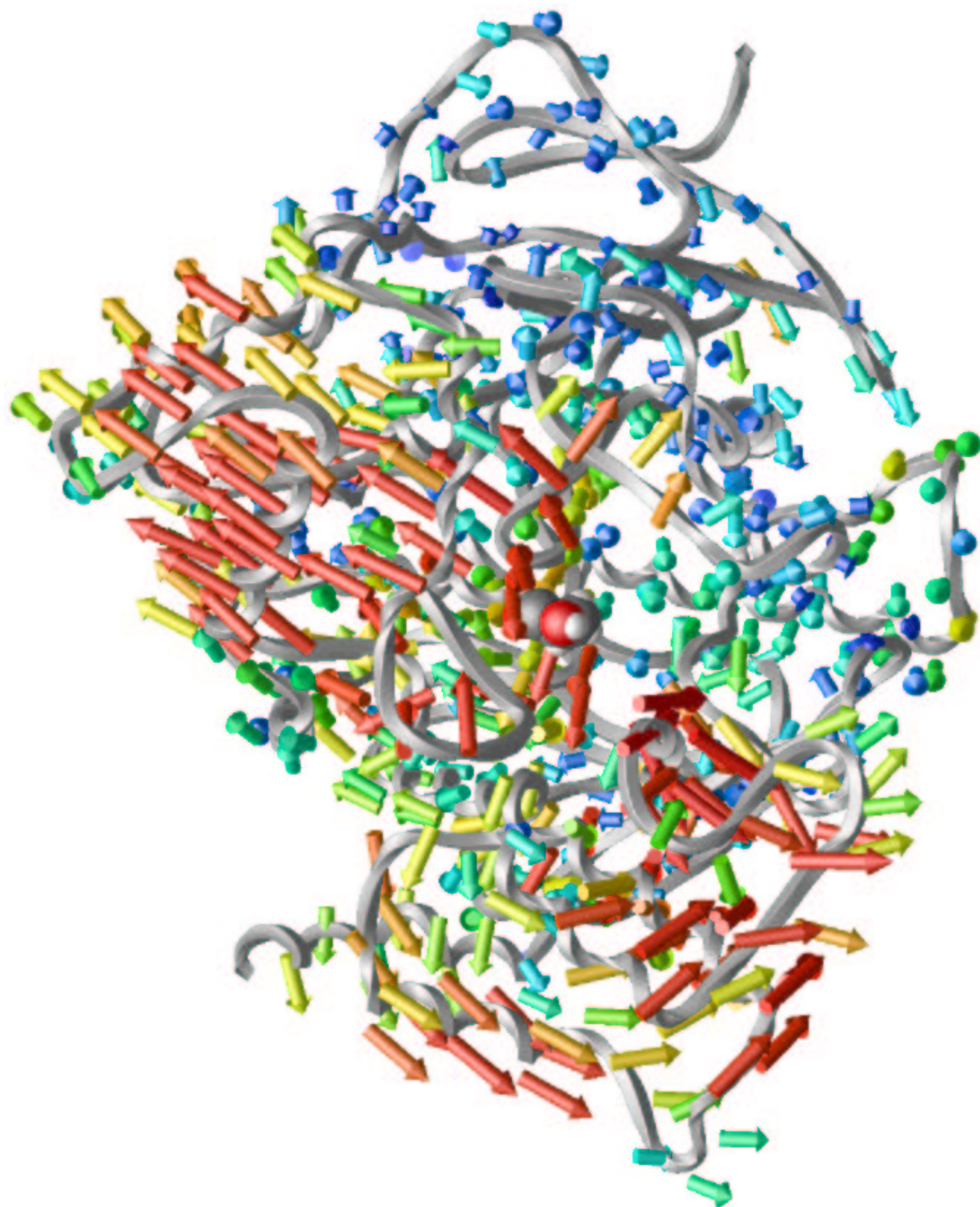


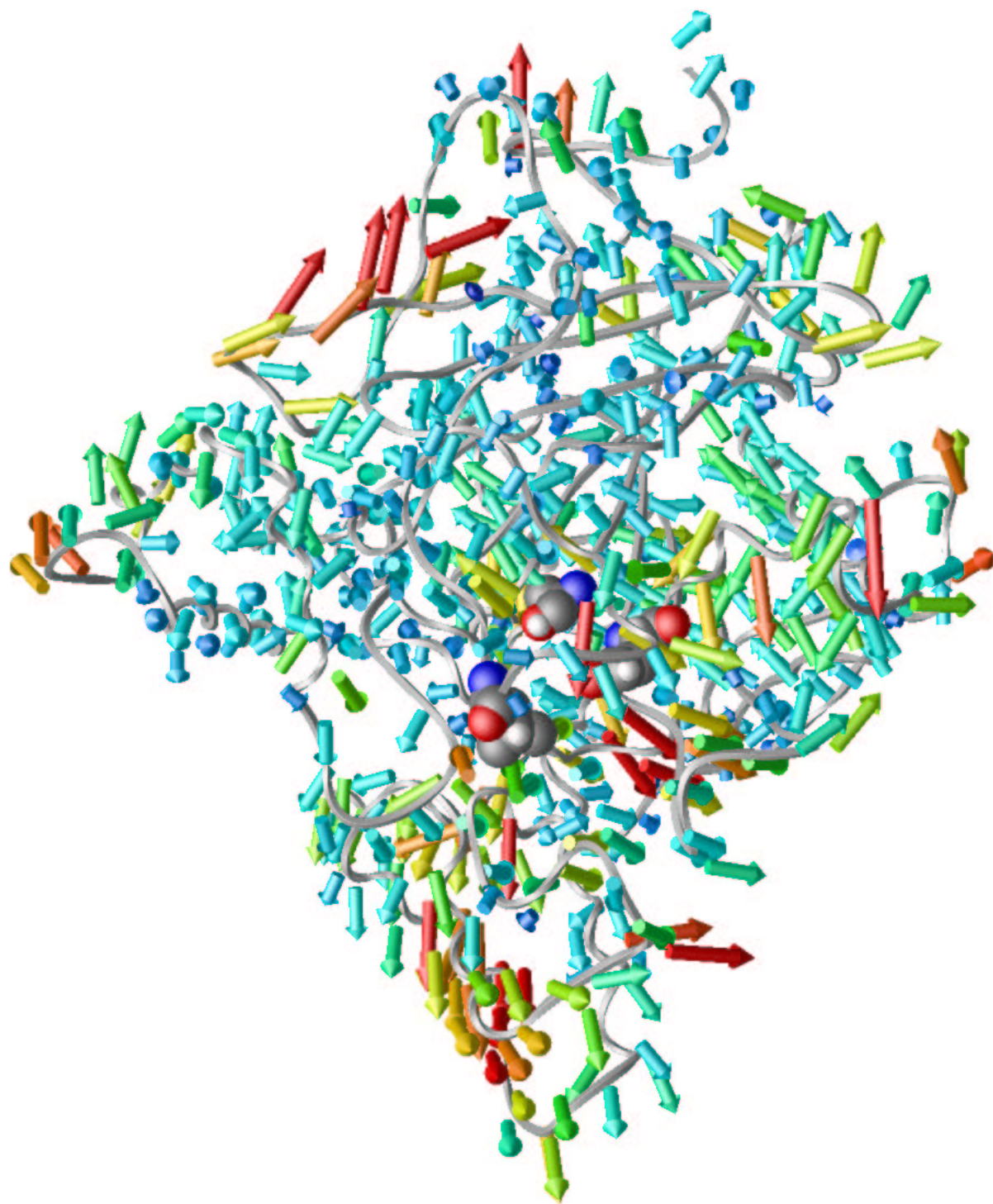




porcupine plot

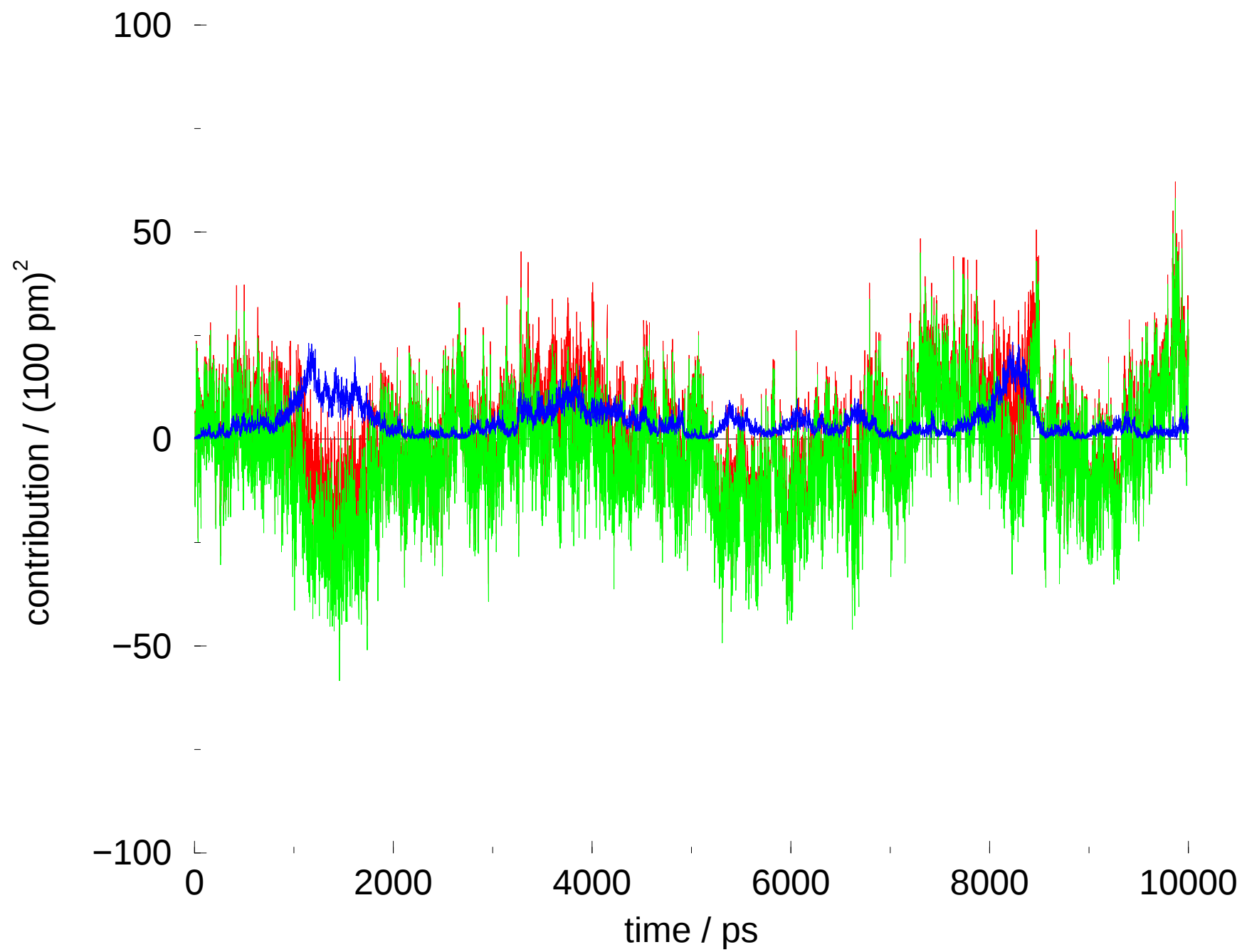
$$\frac{\langle (r_i(t) - \langle r_i \rangle_t) (\rho(t) - \langle \rho \rangle_t) \rangle_t}{\sqrt{\langle (r_i(t) - \langle r_i \rangle_t)^2 \rangle_t \langle (\rho(t) - \langle \rho \rangle_t)^2 \rangle_t}}$$





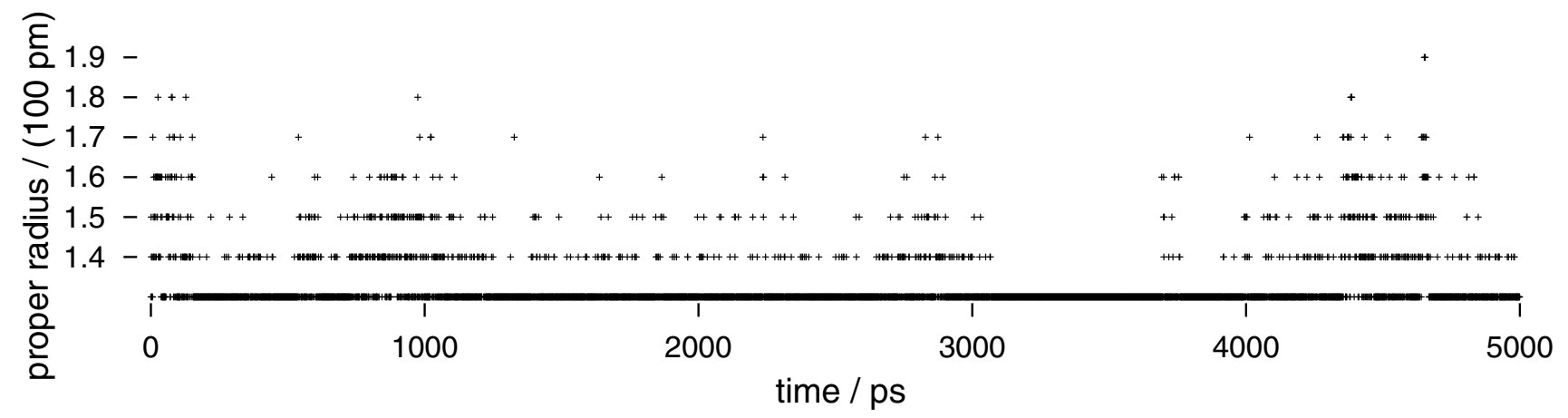
principal component analysis

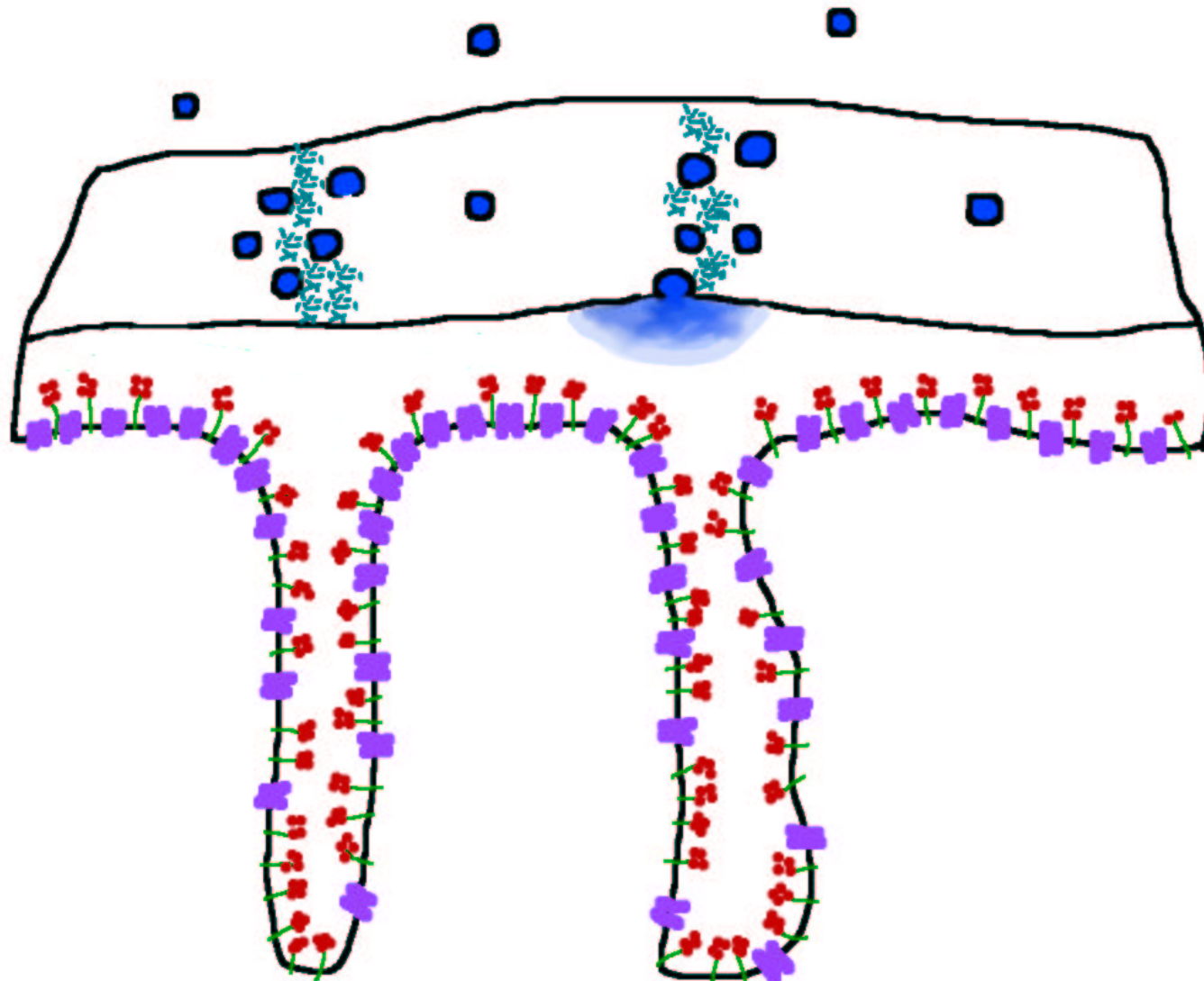
$$\begin{aligned} [\rho(t)]^2 &\approx S \\ &+ \sum_{c=1}^{3N} R_c p_c(t) \\ &+ \sum_{c_1=1}^{3N} \sum_{c_2=1}^{3N} Q_{c_1 c_2} p_{c_1}(t) p_{c_2}(t) \end{aligned}$$

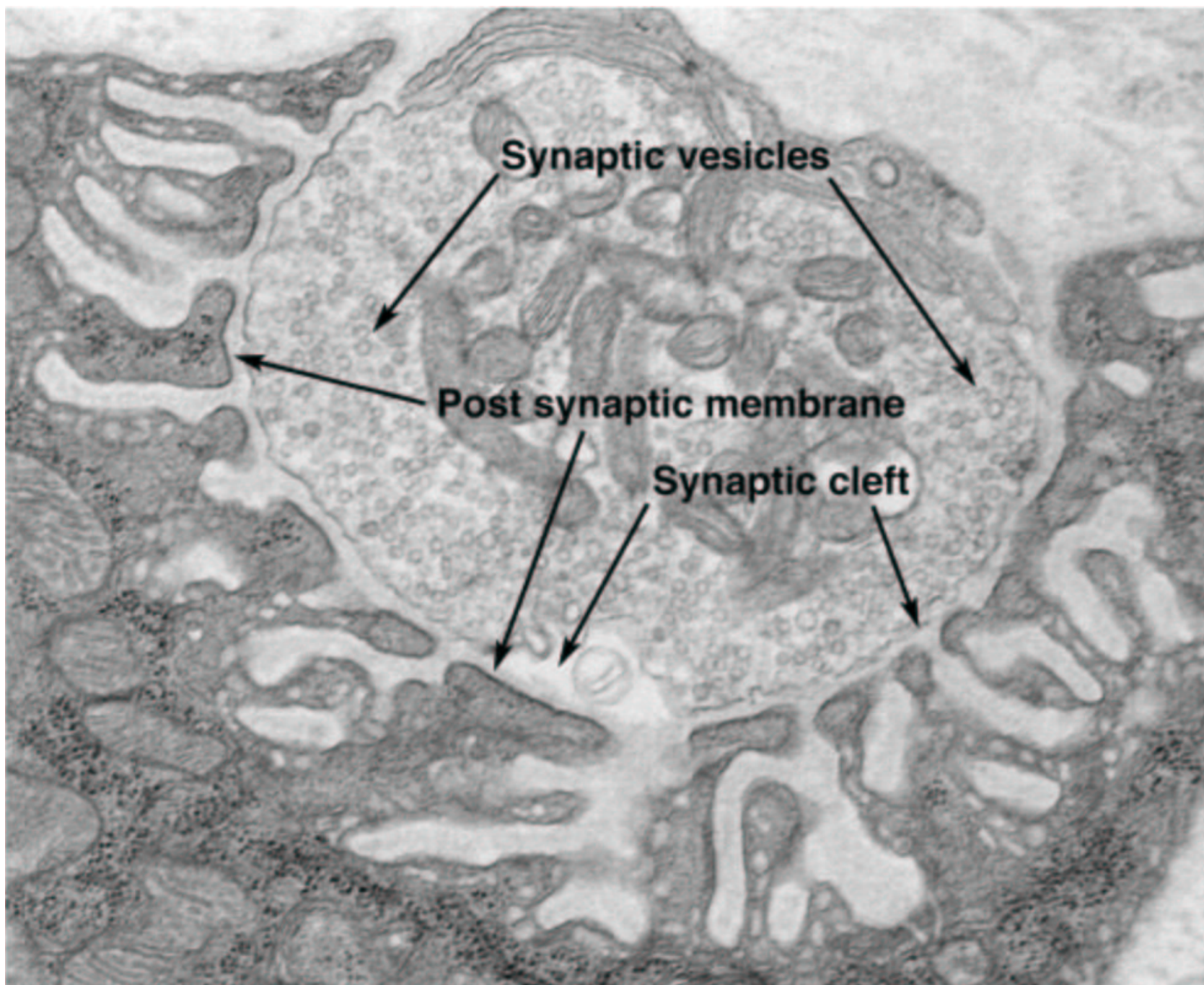


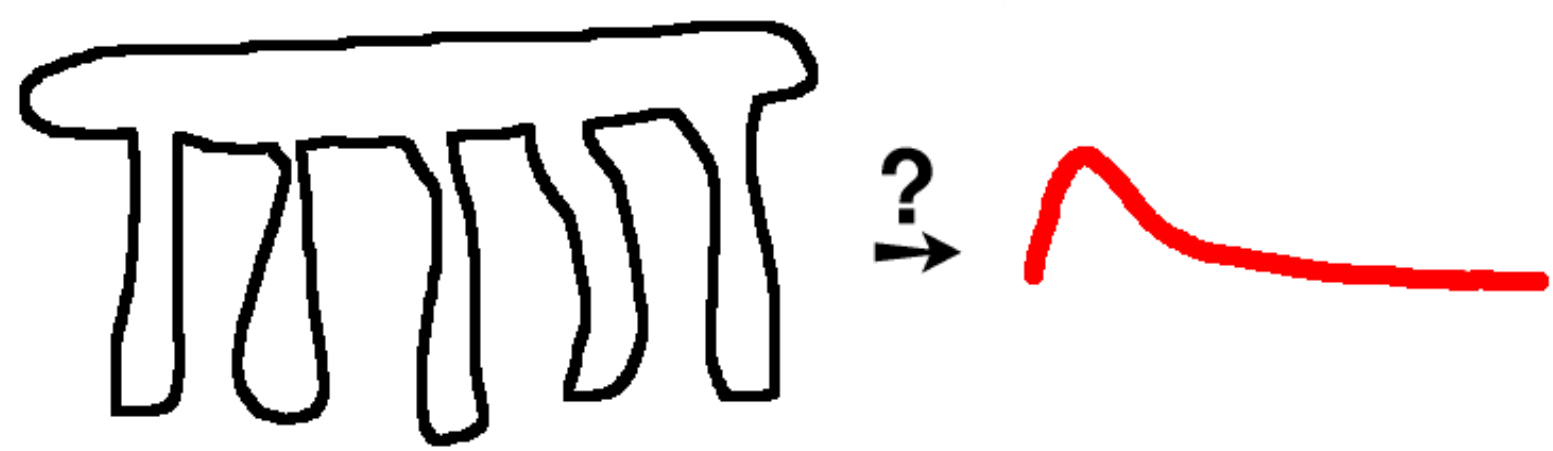
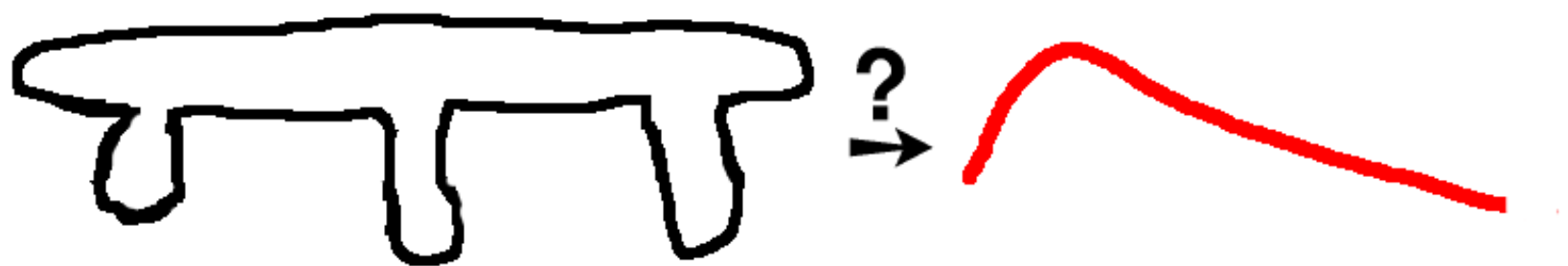


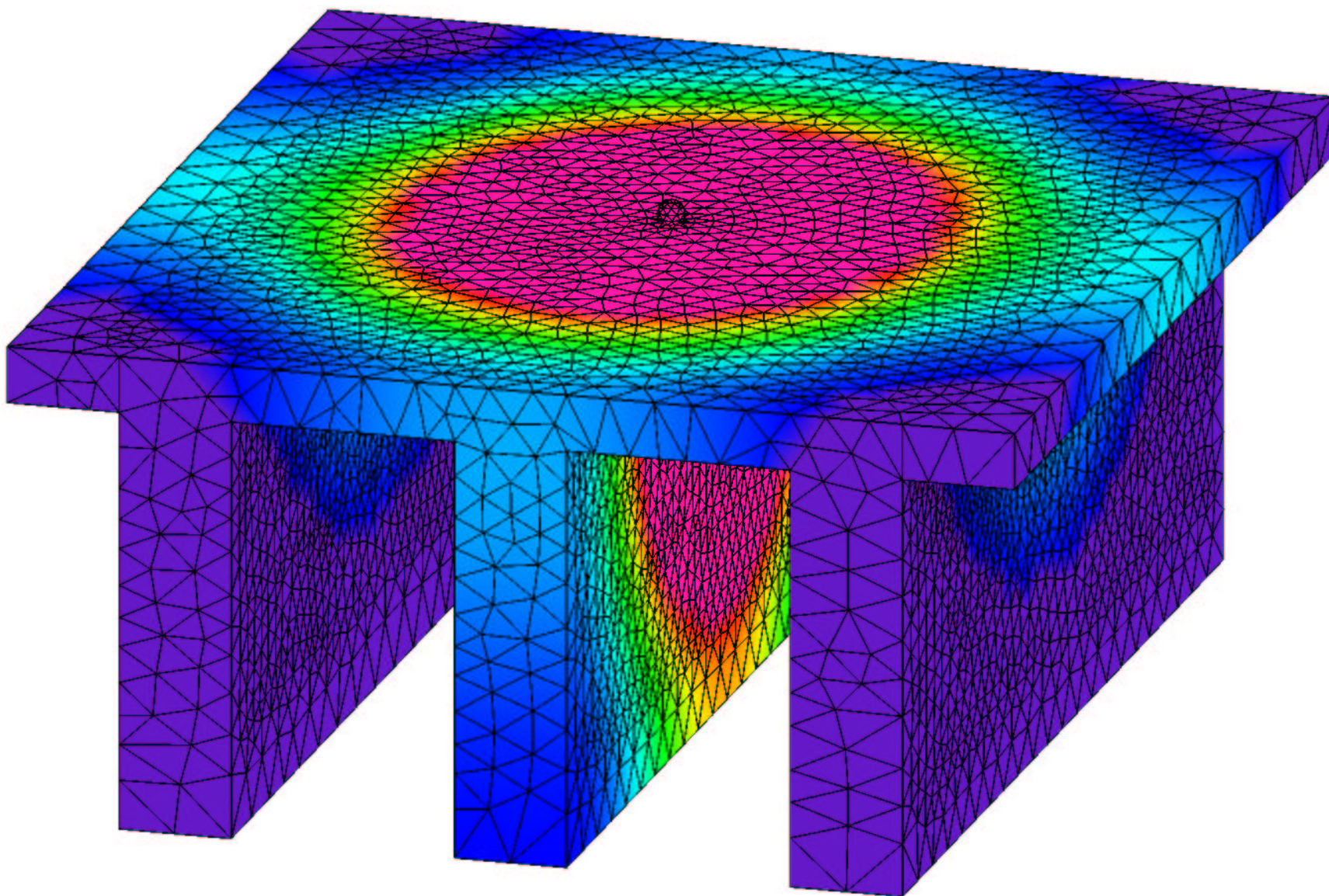
back door

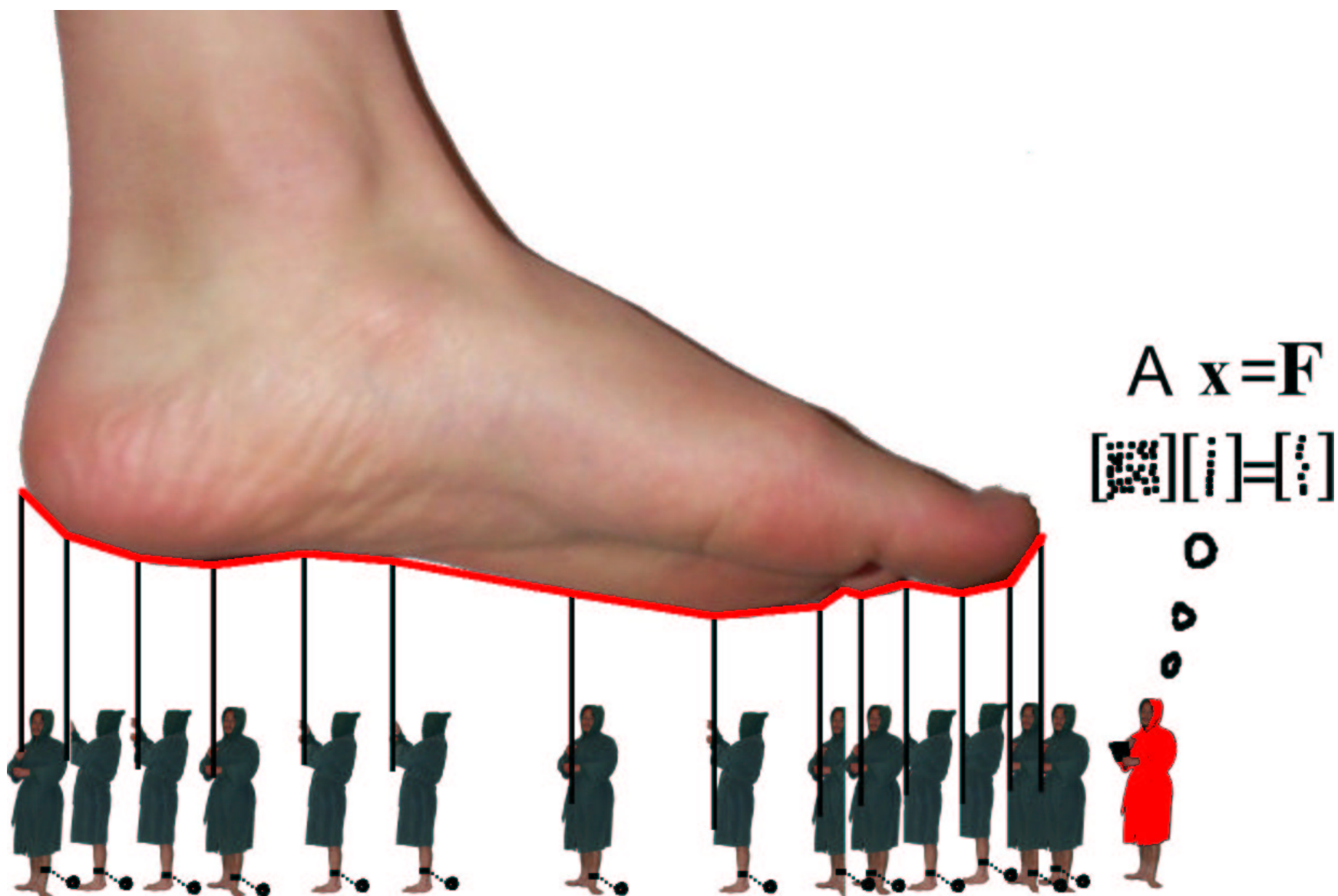


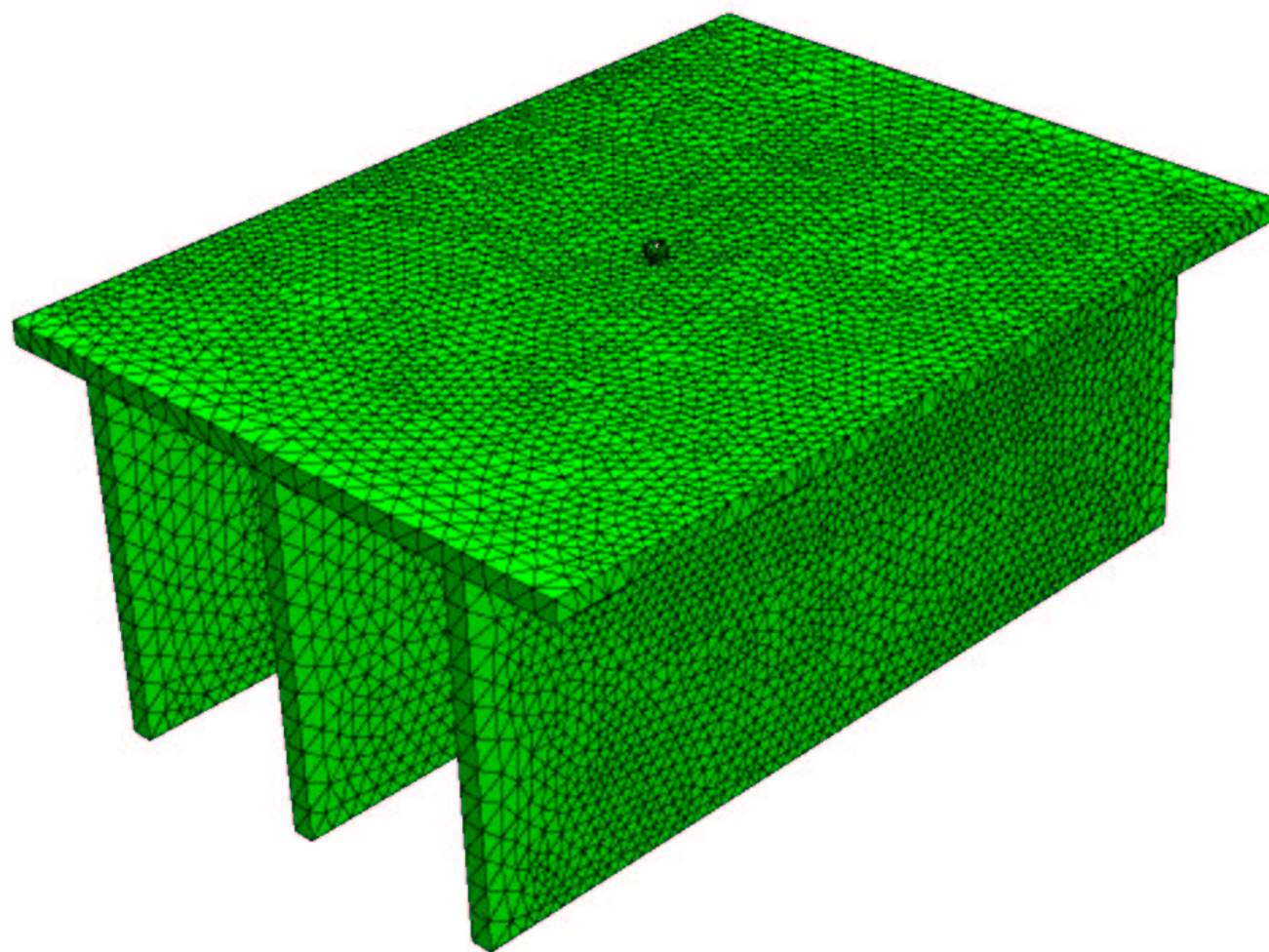


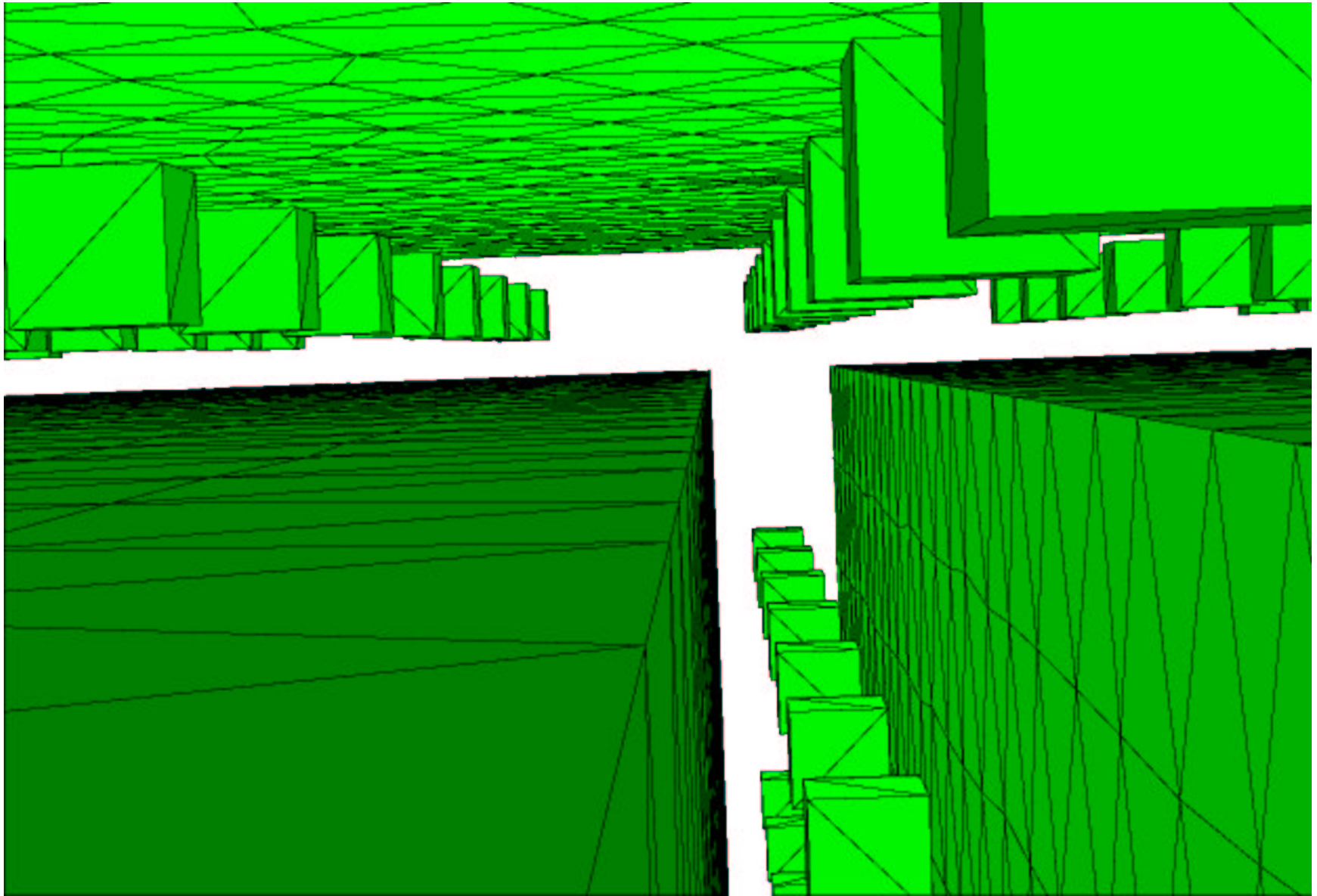


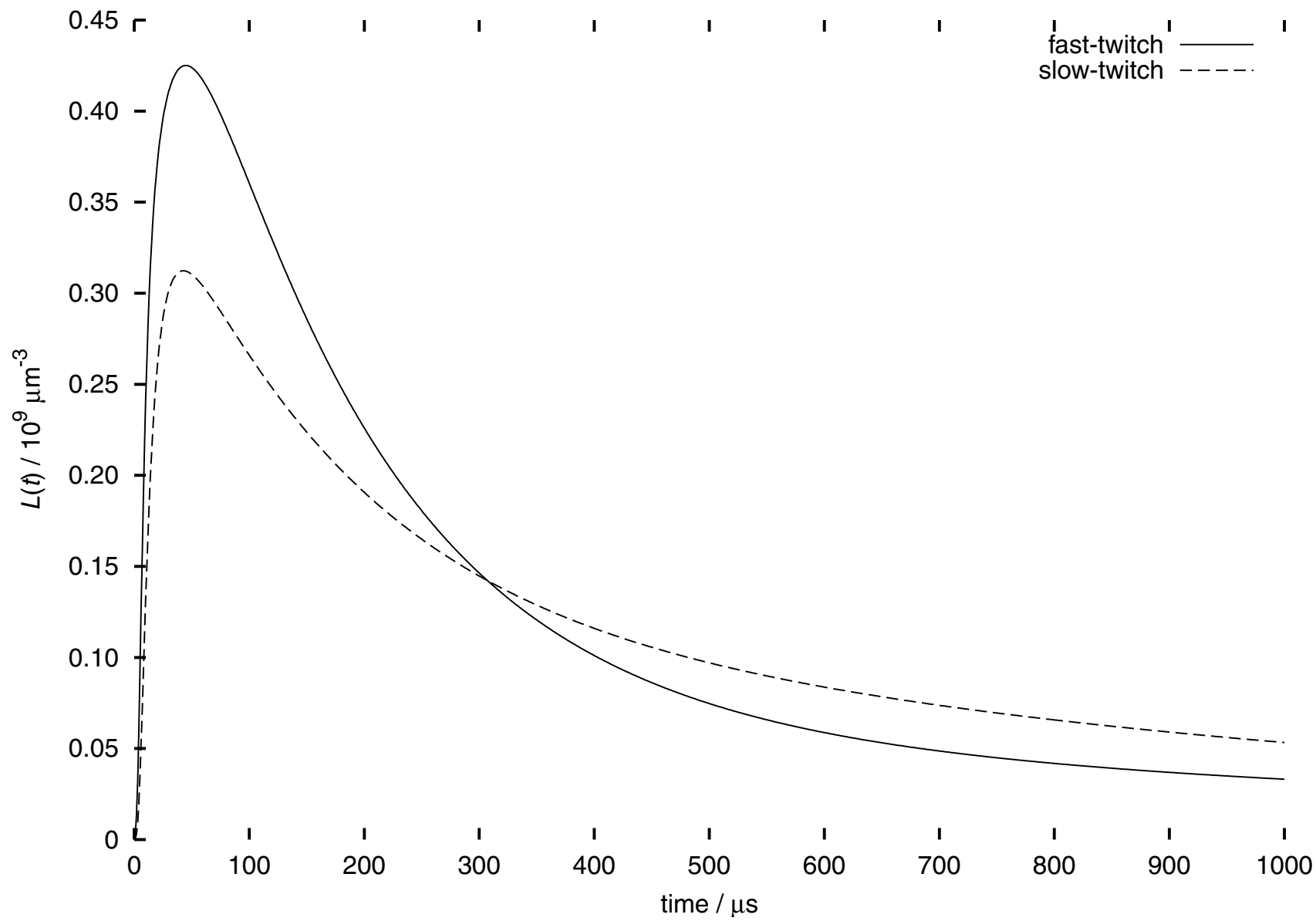


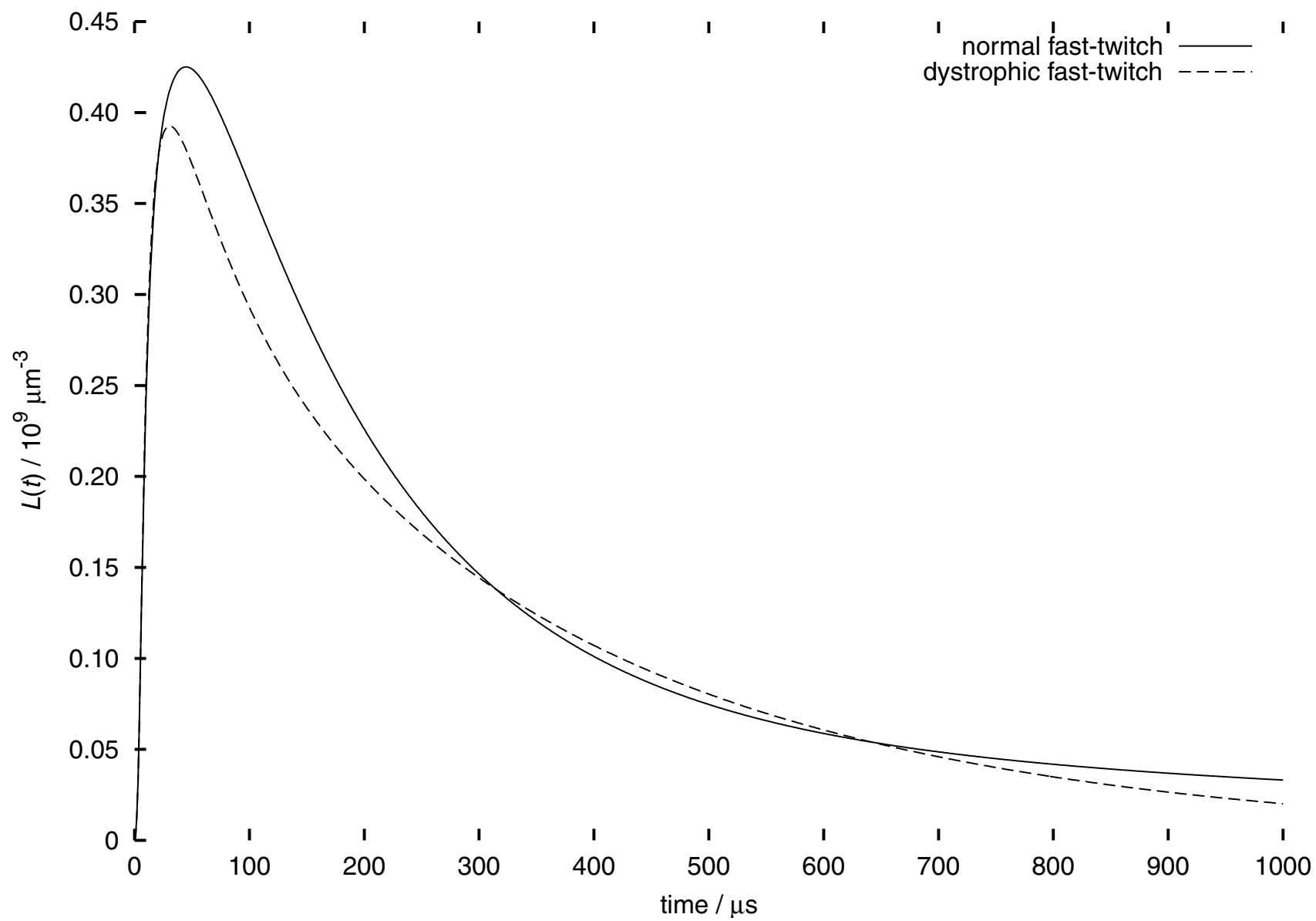


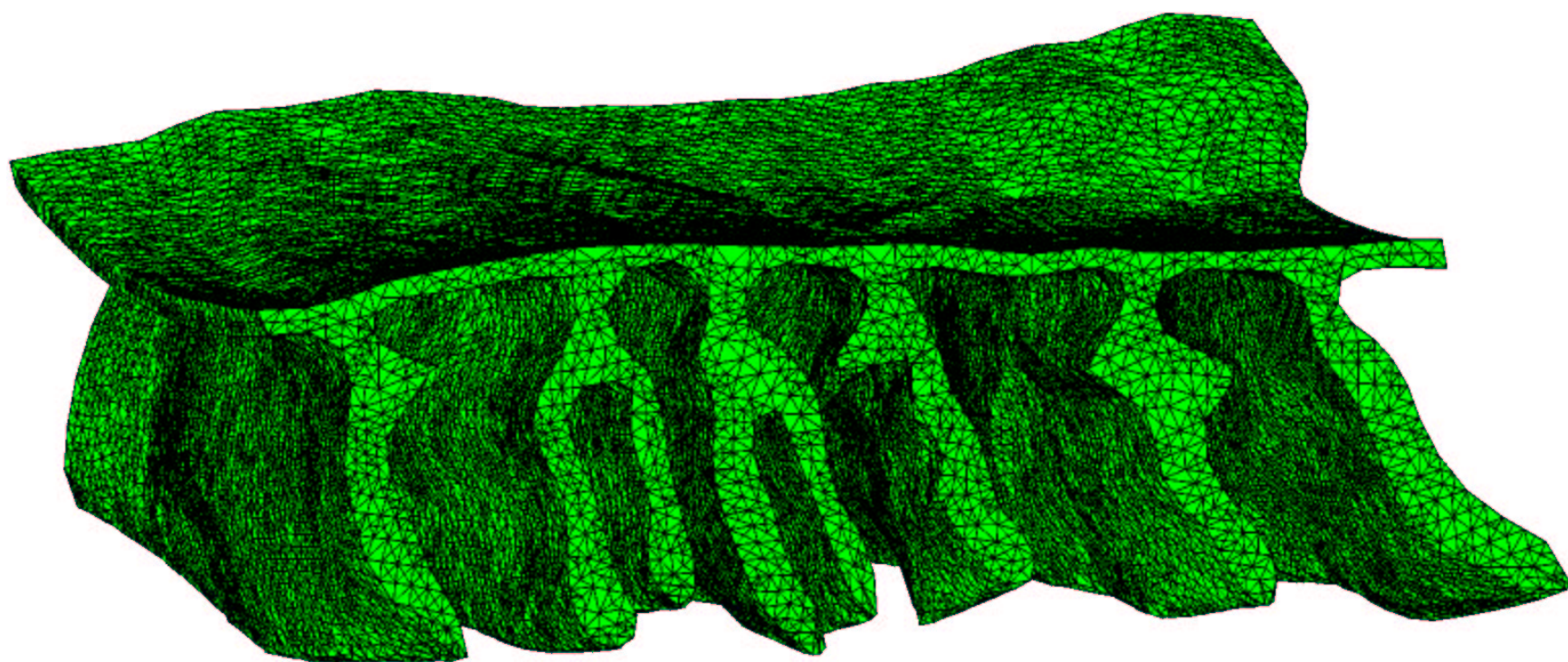


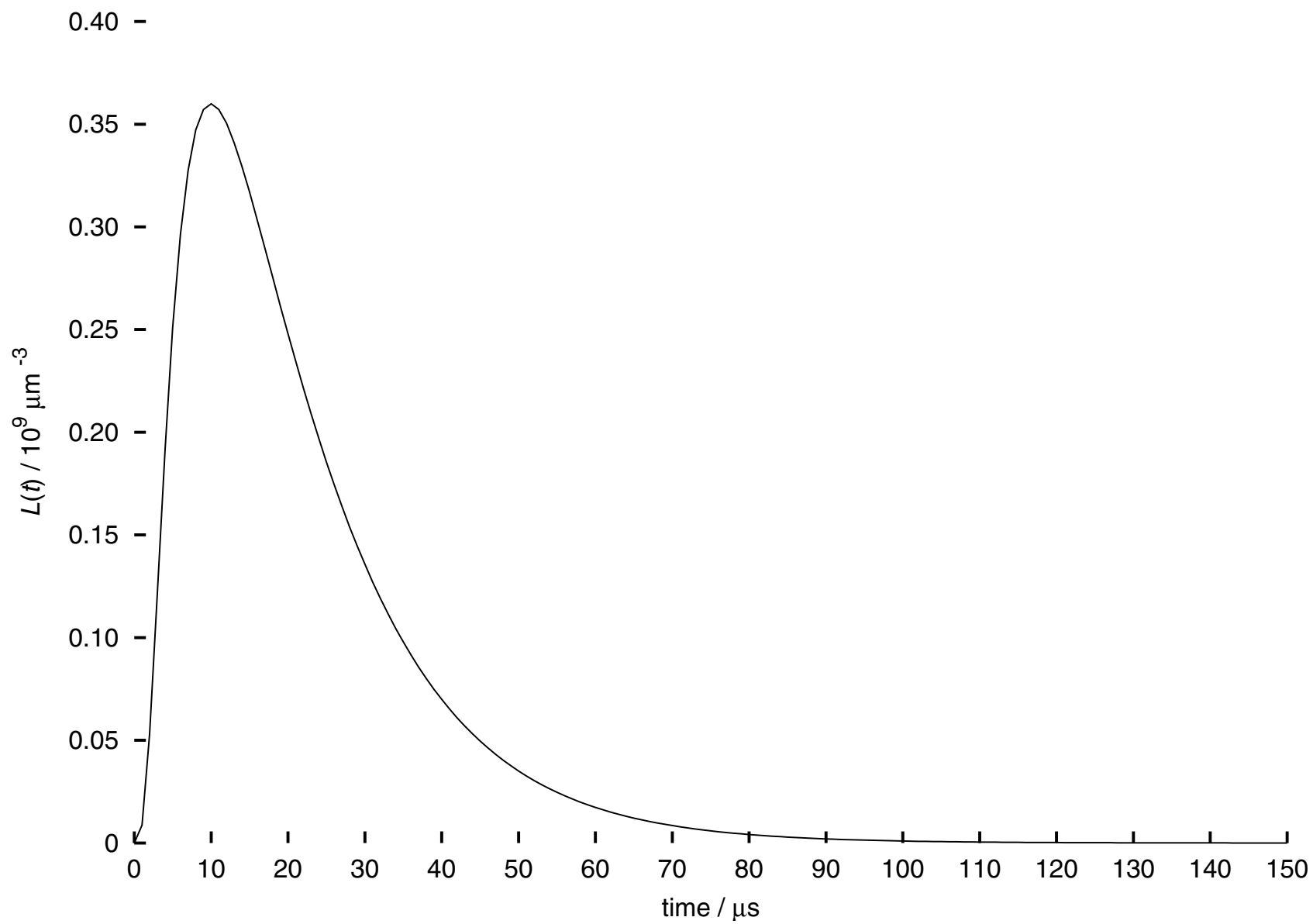












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